total PSI effort. These eukaryotic targets frequently present unique challenges. All CESG protein production protocols and Technology Dissemination Reports are accessible through the PSI Knowledgebase: http://kb-psi-structuralgenomics.org/KB/ and CESG's website. Selected technology developments are presented here. These include advances in expression vector design, enhanced methodology for cell based and wheat germ cell-free expression systems, new software to improve the quality and reduce time for structure determination by X-ray crystallography and NMR, and optimized techniques for the production of TEV protease for use in our protein production platform. We actively share our advances with the biotechnology, pharmaceutical, and academic communities through collaborations, oral presentations, peer-reviewed articles, submissions to public databases and material distribution channels, including PepcDB, PDB, BMRB, PSI Materials Repository, and technology transfer workshops.
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1307-Pos
Effective Protein Crystallization Screening with Synthetic Zeolite Molecular Sieves as Hetero-Epitaxic Nucleant
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Protein crystallization is still a major bottleneck in structural biology. As the current methodology of protein crystallization is a type of screening, it is usually difficult to crystallize important target proteins. The hetero-epitaxial growth from the surface of mineral crystal as a nucleant had been thought to be effective to enhance the chance of protein crystallization. However, generally applicable hetero-epitaxial nucleants for protein crystallization have never been found. Recently, we have reported a protein crystallization method using synthetic zeolite molecular sieves as a hetero-epitaxic nucleant. This method is based on the packing space expansion of protein crystals by a directed nucleation on the material surface, thereby providing new crystal forms with a substantial improvement of diffraction quality in some cases. In this work, a sparse matrix crystallization screening experiment of xylanase from *Trichoderma longibrachiatum* was performed with and without molecular sieves, using a commercially available sparse matrix screening kit. A result of crystallization screening of xylanase showed that molecular sieves promotes the crystallization of xylanase, suggesting that the hetero-epitaxic nucleate approach allows us to improve the effectiveness of the sparse matrix screening of protein crystallization. Interestingly, molecular sieves 5A and 13X provided a new crystal form under the crystallization condition containing zinc, in which a zinc-mediated protein sheet looked favorable for the hetero-epitaxic 3D crystal growth.

1308-Pos
Structural Biology Reveals A New Protein Family from *S.Cerevisiae* with A Novel Fold and Implicated in the Metabolism Control And Drug Resistance
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We have undertaken a small-scale structural genome project focusing on *S. cerevisiae* ORFs without characterized functional motifs or known primary sequence homologs. The cloning, expression and purification screening of 9 targets sequences, led to the determination of the crystal structure of Yer067w by Multiple Anomalous Diffraction at 1.7 Å resolution. This 20 KDa protein present an alpha-beta fold where the 7-stranded beta-sheet is backed by 4 alpha-helices on one side. Interestingly, a structure-based search using the servers SSM or DALI retrieved only proteins with insignificant superposition scores, indicating that Yer067w represents a novel fold superfamily. The phylogenetic analysis of Yer067w primary sequence homologs showed that this protein belongs to a well-conserved family exclusive to Ascomycetes. To further understand Yer067w role we have searched for functional hints using yeast strains deleted for this gene and its paralog *YIL057C*. Microarray analysis of Δyer067w revealed important modifications in expression of genes related to oxidative phosphorylation, amino acids and lipid metabolism. In a screening for phenotypes, we verified that all mutants presented growth deficiencies in non fermentative carbon sources and Western bolt analysis showed that the presence of both proteins are tightly linked to growth on respiratory substrates or low nutrient conditions, suggesting that both proteins are important to the metabolism in glucose free media. Furthermore, Yer067w mutants revealed an antifungal drug resistance phenotype, presenting an increment of 2 times in the MIC for Nystatin and anphotericin B. This work highlights the importance of functional characterization of unknown ORFs for the comprehension of yeast cells metabolism and for uncover new regulatory elements. Support: FAPERJ, CNPq, CIHR

Protein Aggregates I

1309-Pos
Thermodynamic Instability of A Self-Assembled 16-Residue Alanine-Based Oligopeptide in Aqueous Media: Hydrogel, Fibril, and Beaded Filament Formation
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Oligoalanines with greater than ca. 14 residues, which have been doped with charged residues (e.g. lysine), usually adopt α-helical conformations in aqueous media.[1] In contrast, Ac-$(AAKA)_4$-NH_2 aggregates instantaneously when dissolved in aqueous media at concentrations ranging from 70 μM to 7 mM. Evidence from UV circular dichroism (UV-CD) and FTIR spectroscopies suggest a mostly β-sheet like conformation. Kinetics studies of the initially formed conformations suggest a transition from a mostly β-like to a mostly PPII-like conformation, in contrast to typical fibril formation/growth studies. AFM images of freshly prepared samples indicate a porous, tissue-like architecture. Addition of salts (e.g. NaCl) stabilizes this architecture, resulting in the formation of a macroscopic hydrogel. β-sheet and hydrogel formation by such an amino acid sequence is quite unusual, as it does not obey typical rules required for peptide hydrogel formation. In particular, there are no alternating complimentary charges, nor alternating hydrophilic and hydrophobic residues. Without the added stabilization provided by the addition of salts, however, the peptide transitions from a mostly β-sheet-like structure to a PPII-like conformation, possibly via triple helix formation, as evidenced by both electronic and vibrational CD. AFM images suggest the formation of a heterogeneous mixture of assemblies, including bead-like filaments as well as networks of well-defined, intertwined fibrils. Potential applications for peptide hydrogels include drug delivery devices and tissue engineering scaffolds. In this regard, release studies of model peptides which have been trapped within the peptide hydrogel will be presented, as well as rheological characterization of the hydrogel as a function of salt and peptide concentration.
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1310-Pos
The Self-Aggregation of A Polyalanine Octamer Promoted by its C-terminal Tyrosine and Probed by A Strongly Enhanced VCD Signal
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The 8-residue alanine oligopeptide, Ac-A_4KA_2Y-NH_2(AKY8), was found to form amyloid-like fibrils upon incubation at room temperature in acidified aqueous solution, at peptide concentrations > 10 mM. The fibril solution exhibits an enhanced VCD couplet in the amide I' band region, which is nearly 2 orders of magnitude larger than typical polypeptide/protein signals in this region. Such intensity enhancements have recently been observed for insulin and lysozyme fibrils.[1] We performed simulations of the VCD and IR amide I' band profile using a simplified excitonic coupling model. Preliminary results suggest that inter-sheet coupling is responsible for the VCD intensity enhancement. The UV-CD spectrum of the fibril solution shows circular dichroism in the region associated with the tyrosine side chain absorption. A similar peptide, Ac-A_4KA_2-NH_2 (AK7), lacking in a terminal tyrosine residue, does not aggregate. These results suggest a pivotal role for the C-terminal tyrosine residue in stabilizing the aggregation state of this peptide. It is speculated that interactions between the lysine and tyrosine side chains of consecutive strands in an antiparallel arrangement, e.g. via cation-π interactions, are responsible for the stabilization of the resulting fibrils. These results offer considerations and insight for the de novo design of self-assembling oligopeptides for biomedical and biotechnological applications, and highlight the usefulness of VCD as a tool to probe amyloid fibril formation.
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